

Small-scale phase separation in doped anisotropic antiferromagnets

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We analyze the possibility of the nanoscale phase separation manifesting itself in the formation of ferromagnetic (FM) polarons (FM droplets) in the general situation of doped anisotropic three- and two-dimensional antiferromagnets. In these cases, we calculate the shape of the most energetically favorable droplets. We show that the binding energy and the volume of a FM droplet in the three-dimensional (3D) case depend only upon two universal parameters $\bar{J} = (J_x + J_y + J_z)S^2$ and $t_{eff} = (t_x t_y t_z)^{1/3}$, where \bar{J} and t_{eff} are effective antiferromagnetic (AFM) exchange and hopping integrals, respectively. In the two-dimensional (2D) case, these parameters have the form $\bar{J} = (J_x + J_y)S^2$ and $t_{eff} = (t_x t_y)^{1/2}$. The most favorable shape of a ferromagnetic droplet corresponds to an ellipse in the 2D case and to an ellipsoid in the 3D case.

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I. INTRODUCTION

The problem of electronic phase separation with the formation of ferromagnetic (FM) or paramagnetic (PM) spin polarons (magnetic droplets or ferrons) due to the self-trapping of charge carriers in an antiferromagnetic (AFM) matrix became very popular nowadays, especially in the studies of high- T_c superconductors and the systems with the colossal magnetoresistance (such as LaMnO_3 manganites doped by Ca). For isotropic materials, the size and shape of FM droplets was evaluated in several papers beginning from the seminal work of Nagaev¹, for more detail see Ref. 2. The characteristic size of a FM droplet turns out to be of the order of 15–20 Å and its optimum shape in isotropic 3D manganites is a spherical one. Later on, Kagan and Kugel³ analyzed the case of layered manganites (like $(\text{La,Ca})_{n+1}\text{Mn}_n\text{O}_{3n+1}$) and demonstrated that the droplets with the lowest energy have the ellipsoidal shape. The FM droplets of cylindrical shape considered first by Nagaev⁴ for this class of manganites correspond to a higher energy. Currently, the phase separation in anisotropic materials was also addressed in connection with low-dimensional organic compounds⁵ and quasi-one-dimensional magnets such as BaCoO_3 ^{6,7}. Magnetic polarons in doped one-dimensional (1D) AFM magnetic chains were recently considered in Refs. 8,9,10, where the possibility of rather long-range magnetic distortions around the polaron was demonstrated.

Another possibility to have a strongly anisotropic situation arises when we take into account an interplay between the microscopic phase separation and charge ordering (stripe formation), include the Jahn-Teller type

of effects (orbital degrees of freedom), or consider stable crystallographic distortions. In these cases, the quasi-1D zig-zag or ladder structures are often observed in the corresponding systems^{11,12}.

In this paper, we present the calculations concerning the shape and size of FM droplets in anisotropic two-dimensional (2D) or three-dimensional (3D) cases when, generally speaking, the electron hopping integrals t_x , t_y , and t_z along x , y , and z directions, as well as the AFM exchange integrals J_x , J_y , and J_z are different. We get that, by analogy with the situation in layered manganites³, the most favorable shape of a FM droplet is an ellipsoidal one. Moreover, the binding energy and the effective volume of the droplet are expressed only in terms of universal averaged parameters $\bar{J} = (J_x + J_y + J_z)S^2$ and $t_{eff} = (t_x t_y t_z)^{1/3}$. These results are interesting, in particular, in relation to the neutron scattering experiments giving an indication of the existence of FM clusters with different shapes in perovskite and layered manganites^{13,14,15}.

Our paper is organized as follows. First, we consider the purely 2D situation and find the most favorable shape of a 2D ferron comparing the energies of elliptical and rectangular droplets in the general anisotropic 2D case: $t_x \neq t_y$ and $J_x \neq J_y$. We find that in two dimensions, the minimal energy corresponds to the elliptical shape. Then, we include the third dimension (J_z and t_z) and compare the energies of the cylinder and ellipse in the case when both of them have the optimum elliptical shape of the 2D cross-sections. We find again that the minimal energy in the 3D case corresponds to the ellipsoidal shape of FM droplets. At the end of the paper, we provide some discussions and conclusions.

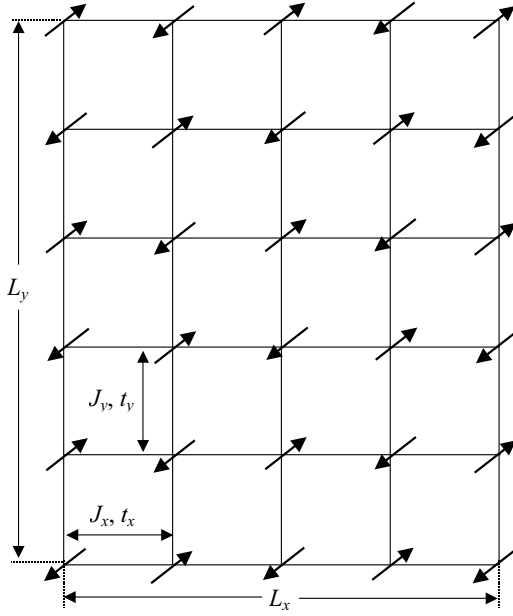


Figure 1: 2D anisotropic doped antiferromagnet with the square lattice. $J_x \neq J_y$ are AFM exchange integrals, $t_x \neq t_y$ are the electron hopping integrals, L_x and L_y define the volume of the rectangular ferron in 2D.

II. THE SHAPE OF FM DROPLETS IN THE ANISOTROPIC 2D CASE

Let us first consider the anisotropic 2D case. In this case, there are two different electron hopping integrals $t_x \neq t_y$ and two different constants of the AFM exchange interaction $J_x \neq J_y$, see Fig. 1. To some extent, this case has a lot of similarities with two-leg ladder systems rather popular nowadays (see, for example, Ref. 16 and references therein).

Throughout this paper, we consider the Kondo-lattice model with the Hamiltonian

$$\hat{H} = J_H \sum_i \mathbf{S}_i \sigma_i + \sum_{\langle ij \rangle_\alpha} J_\alpha \mathbf{S}_i \mathbf{S}_j + \sum_{\langle ij \rangle_\alpha} t_\alpha c_i^\dagger c_j, \quad (1)$$

where, c_i^\dagger and c_i are electron creation and annihilation operators at site i , $\alpha = \{x, y\}$ for a square lattice in 2D, $\langle ij \rangle_\alpha$ denote the neighboring sites in the lattice along the α direction, $\sigma_i = c_i^\dagger \sigma c_i$ is the spin of a conduction electron (σ is the Pauli matrix), \mathbf{S}_i is a local spin, J_α are AFM exchange integrals, t_α are the hopping integrals for conduction electrons, and parameter J_H corresponds to the Hund's rule coupling between a local spin \mathbf{S} and a spin of a conduction electron.

We work in the double-exchange limit, which implies that $J_H \gg \{t_x, t_y\} \gg \{J_x, J_y\}$. In this case, the ground state of the system is unstable toward the nanoscale phase separation^{1,2,3} with the formation of FM polarons inside the AFM matrix. Let us now evaluate the total energy of the phase-separated state for different shapes of ferrons possible in the 2D case.

A. A rectangular ferron

Let us first consider a rectangular FM droplet (ferron) located at the square lattice with the intersite distance a . Its characteristic sizes along x and y axes are L_x and L_y , respectively. The dimensionless volume Ω of such a ferron can be defined as $\Omega = L_x L_y / a^2$. The kinetic energy of charge carriers (electrons or holes) within the FM droplet is

$$E_{kin} = -2t_x n - 2t_y n + \varepsilon_0 n, \quad (2)$$

where n is the concentration of charge carriers and ε_0 is a binding energy corresponding to the first (the lowest) level in the rectangular potential well. The latter can be found by solving the corresponding Schrödinger equation (see Ref.3)

$$\hat{H}_{kin} \Psi(x, y) = \varepsilon_0 \Psi(x, y), \quad (3)$$

where

$$\hat{H}_{kin} = -a^2 \left(t_x \frac{\partial^2}{\partial x^2} + t_y \frac{\partial^2}{\partial y^2} \right). \quad (4)$$

For the case of a well-defined ferron (without an extended tail of magnetic distortions, which we will consider throughout the present paper, the corresponding boundary conditions have the form

$$\Psi(x = L_x, y) = \Psi(x, y = L_y) = 0. \quad (5)$$

Hence,

$$\Psi(x, y) = \sin \frac{\pi x}{L_x} \sin \frac{\pi y}{L_y} \quad (6)$$

and

$$\varepsilon_0 = t_x \left(\frac{\pi a}{L_x} \right)^2 + t_y \left(\frac{\pi a}{L_y} \right)^2. \quad (7)$$

Now, we can pass to the evaluation of the potential energy given by the terms related to the AFM exchange interaction. In the domains with the ferromagnetic order (ferrons), the AFM exchange leads to the positive contribution to the total energy

$$E_{pot1} = 2(J_x + J_y) S^2 n \frac{L_x L_y}{a^2}. \quad (8)$$

For the AFM regions, which are free of ferrons, the corresponding contribution to the energy can be written as

$$E_{pot2} = -2(J_x + J_y) S^2 \left(1 - n \frac{L_x L_y}{a^2} \right). \quad (9)$$

Hence, the total potential energy yields

$$E_{pot} = -2(J_x + J_y) S^2 + 4(J_x + J_y) S^2 n \frac{L_x L_y}{a^2}. \quad (10)$$

As a result, the total energy related to the formation of FM droplets has the following form

$$E_{tot} = -2 [t_x n + t_y n + (J_x + J_y) S^2] + n \left[t_x \left(\frac{\pi a}{L_x} \right)^2 + t_y \left(\frac{\pi a}{L_y} \right)^2 \right] + 4 (J_x + J_y) S^2 n \frac{L_x L_y}{a^2}. \quad (11)$$

The minimization of energy (11) with respect to L_x and L_y gives

$$\begin{aligned} \frac{\partial E_{tot}}{\partial L_x} &= -2nt_x \frac{\pi^2 a^2}{L_x^3} + 4(J_x + J_y) n S^2 \frac{L_y}{a^2} = 0, \\ \frac{\partial E_{tot}}{\partial L_y} &= -2nt_y \frac{\pi^2 a^2}{L_y^3} + 4(J_x + J_y) n S^2 \frac{L_x}{a^2} = 0. \end{aligned} \quad (12)$$

A solution to equations (12) reads

$$\begin{aligned} t_x \pi^2 &= 2 \frac{L_y L_x^3}{a^4} (J_x + J_y) S^2, \\ t_y \pi^2 &= 2 \frac{L_x L_y^3}{a^4} (J_x + J_y) S^2. \end{aligned} \quad (13)$$

Multiplying two equations (13) by each other, we find

$$\left(\frac{L_y L_x}{a^2} \right)^4 = \frac{\pi^4 t_x t_y}{4 (J_x + J_y)^2 S^4}. \quad (14)$$

Now, introducing notation

$$t_{eff} = (t_x t_y)^{1/2}, \quad \bar{J} = (J_x + J_y) S^2, \quad (15)$$

we find

$$\left(\frac{L_y L_x}{a^2} \right)^4 = \Omega^4 = \frac{\pi^4 t_{eff}^2}{4 \bar{J}^2}.$$

Thus, the dimensionless volume (area) Ω of a 2D ferron can be written as

$$\Omega = \frac{\pi}{\sqrt{2}} \left(\frac{t_{eff}}{\bar{J}} \right)^{1/2}. \quad (16)$$

We get quite a remarkable relationship expressing the volume of a 2D ferron in terms of the t_{eff}/\bar{J} ratio.

Correspondingly, the minimized total energy (11) takes the form

$$E_{tot} = -2 (t_x n + t_y n + \bar{J}) + 4\pi\sqrt{2}n (t_{eff}\bar{J})^{1/2}. \quad (17)$$

Introducing the energy of FM polaron by the relationship

$$E_{pol} = E_{tot} + 2 (t_x n + t_y n + \bar{J}), \quad (18)$$

we get finally

$$E_{pol} = 8n\Omega\bar{J} = 4\pi\sqrt{2}n (t_{eff}\bar{J})^{1/2}. \quad (19)$$

It is again worth to notice that the energy of the FM polaron in 2D depends only upon the product of t_{eff} and \bar{J} .

B. An elliptical ferron

Now, we can consider the energy a two-dimensional FM polaron having the shape of an ellipse. For the same characteristic sizes (principal axes) of the ferron, its volume in the case of an ellipse is $\Omega = \pi L_x L_y / a^2$. The corresponding kinetic energy is again given by Eqs. (2)-(4). To solve the Schrödinger equation in this geometry, we should transform an ellipse to a circle. This could be done, for example, by the dilatation along the y axis: $y = \tilde{y} \sqrt{t_y/t_x}$. Then, we have

$$\hat{H}_{kin} = -a^2 t_x \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial \tilde{y}^2} \right) = -a^2 t_x \Delta_{\tilde{R}}, \quad (20)$$

where and $\tilde{R}^2 = x^2 + \tilde{y}^2$ and $\Delta_{\tilde{R}} = \frac{\partial^2}{\partial \tilde{R}^2} + \frac{1}{\tilde{R}} \frac{\partial}{\partial \tilde{R}}$ is the radial part of the Laplacian operator in 2D. Thus, the ellipse $x^2/L_x^2 + y^2/L_y^2 = 1$ in the 'old' x, y coordinates transforms to the $x^2 + \tilde{y}^2 = \tilde{R}_{max}^2$ circle in the 'new' x, \tilde{y} coordinates. From equation for the circle in terms of 'new' coordinates x, \tilde{y} , it is clear that $\tilde{R}_{max} = L_x$. Hence, we have

$$L_x = L_y \sqrt{\frac{t_x}{t_y}} = \tilde{R}_{max}, \quad (21)$$

and the ferron volume in the initial ('old') coordinates reads

$$\Omega = \pi \frac{L_x L_y}{a^2} = \pi \frac{L_x^2}{a^2} \sqrt{\frac{t_y}{t_x}} \quad (22)$$

In this case, a solution to the Schrödinger equation (3) has the form $\Psi = J_0(k\tilde{R})$, where J_0 is the Bessel function of zeroth order. The boundary condition $J_0(k\tilde{R}_{max}) = 0$ yields $k\tilde{R}_{max} = j_{0,1} = 2.404 \approx 3\pi/4$, where $j_{0,1}$ is the first zero of function J_0 . This means that

$$\varepsilon_0 = t_x a^2 k^2 = t_x \left(\frac{j_{0,1} a}{\tilde{R}_{max}} \right)^2 = t_x \left(\frac{j_{0,1} a}{L_x} \right)^2. \quad (23)$$

Then, we have

$$E_{tot} = -2 [t_x n + t_y n + (J_x + J_y) S^2] + E_{pol}, \quad (24)$$

where

$$E_{pol} = n \left(\frac{j_{0,1} a}{L_x} \right)^2 t_x + 4 (J_x + J_y) S^2 n \frac{\pi L_x^2}{a^2} \sqrt{\frac{t_y}{t_x}}. \quad (25)$$

The minimization of polaron energy (25) with respect to L_x gives

$$\frac{\partial E_{pol}}{\partial L_x} = -2nt_x \frac{j_{0,1}^2 a^2}{L_x^3} + 8 (J_x + J_y) S^2 n \frac{\pi L_x}{a^2} \sqrt{\frac{t_y}{t_x}} = 0. \quad (26)$$

Thus, we have (see Eqs. (22) and (26))

$$\Omega^2 = \pi^2 \frac{L_x^4 t_y}{a^4 t_x} = \frac{\pi j_{0,1}^2 t_x}{4(J_x + J_y) S^2} \sqrt{\frac{t_y}{t_x}} \quad (27)$$

Introducing again t_{eff} and \bar{J} defined by Eq. (15), we find

$$\Omega = \frac{j_{0,1} \sqrt{\pi}}{2} \left(\frac{t_{eff}}{\bar{J}} \right)^{1/2}. \quad (28)$$

So, the ferron volume is again expressed as a function of the universal ratio t_{eff}/\bar{J} . Comparing expressions (16) and (28) for the volumes of rectangular and elliptical ferrons, we find

$$\frac{\Omega_{ellipse}}{\Omega_{rectangle}} = \frac{j_{0,1}}{\sqrt{2\pi}} \simeq 0.96 < 1. \quad (29)$$

This means that the elliptical ferron is a more compact object (i.e. it has a smaller volume) in comparison to the rectangular ferron. Accordingly, the energy of elliptical magnetic polaron can be written in the following form

$$E_{pol} = 8n\Omega\bar{J} = 4nj_{0,1}\sqrt{\pi} (t_{eff}\bar{J})^{1/2}. \quad (30)$$

We can see again that the ferron energy depends only upon the product of t_{eff} and \bar{J} . Finally, we can compare the ferron energies for the cases of rectangular and elliptical shapes using Eqs. (19) and (30)

$$\frac{E_{pol}^{ellipse}}{E_{pol}^{rectangle}} = \frac{j_{0,1}}{\sqrt{2\pi}} = \frac{\Omega_{ellipse}}{\Omega_{rectangle}} \simeq 0.96 < 1 \quad (31)$$

We see that the ratio of energies turns out to be identical to the ratio of the volumes. Thus, the elliptical shape of the ferron is more favorable in energy than the rectangular shape. First of all, this is caused by a more compact structure of the elliptical ferron. Another cause was emphasized in Ref. 3. The thing is that the elliptical shape of ferron in 2D has a close similarity to the one-electron spectrum characteristic of the empty square lattice: $\varepsilon_p = p_x^2/2m_x + p_y^2/2m_y$, where $m_x/2 = t_x a^2$ and $m_y/2 = t_y a^2$. Concluding this section, we can say that the elliptical shape is the shape most favorable in energy for a FM droplet in doped anisotropic antiferromagnets with the 2D square lattice.

III. THE SHAPE OF FM DROPLETS IN THE ANISOTROPIC 3D CASE

Now, we can include the third dimension (which means the inclusion of J_z and t_z) and consider the shape of a FM droplet in a doped anisotropic antiferromagnet with the 3D cubic lattice. Of course (having in mind the results of the previous section), we have to consider FM droplets with the 2D cross-section most favorable in energy. In other words, we consider the 3D droplets having the shape of an ellipse in the x, y plane. Then the

problem effectively reduces to the comparison of energies and volumes of a cylinder and of an ellipsoid of rotation both having an elliptical cross-section with dimensions $L_x = L_y \sqrt{\frac{t_x}{t_y}}$ (see Eq. (21)).

A. FM droplets of cylindrical shape

First, let us consider 3D FM droplets of cylindrical shape. The volume of such a droplet can be written as

$$\Omega = \pi \frac{L_x L_y L_z}{a^3} = \pi \frac{L_x^2}{a^2} \sqrt{\frac{t_y}{t_x}} \frac{L_z}{a}. \quad (32)$$

In this case, the total energy has the form

$$E_{tot} = -2 [t_x n + t_y n + t_z n + (J_x + J_y + J_z) S^2] + 4(J_x + J_y + J_z) S^2 \Omega n + t_x n \left(\frac{j_{0,1} a}{L_x} \right)^2 + t_z n \left(\frac{\pi a}{L_z} \right)^2 \quad (33)$$

The polaron energy

$$E_{pol} = E_{tot} + 2 [t_x n + t_y n + t_z n + (J_x + J_y + J_z) S^2] \quad (34)$$

is given by the expression

$$E_{pol} = t_x n \left(\frac{j_{0,1} a}{L_x} \right)^2 + t_z n \left(\frac{\pi a}{L_z} \right)^2 + 4(J_x + J_y + J_z) S^2 n \pi \frac{L_x^2}{a^2} \sqrt{\frac{t_y}{t_x}} \frac{L_z}{a}. \quad (35)$$

The minimization of polaron energy (35) with respect to L_x and L_z yields

$$\begin{aligned} \frac{\partial E_{pol}}{\partial L_x} &= -2t_x n \frac{j_{0,1}^2 a^2}{L_x^3} + 8\bar{J} n \pi \frac{L_x}{a^2} \frac{L_z}{a} \sqrt{\frac{t_y}{t_x}} = 0, \\ \frac{\partial E_{pol}}{\partial L_z} &= -2t_z n \frac{\pi^2 a^2}{L_z^3} + 4\bar{J} n \pi \frac{L_x^2}{a^3} \sqrt{\frac{t_y}{t_x}} = 0. \end{aligned} \quad (36)$$

where we introduced the effective exchange integral for the 3D case

$$\bar{J} = (J_x + J_y + J_z) S^2, \quad (37)$$

From Eqs. (36), we get

$$\begin{aligned} \frac{j_{0,1}^2 t_x}{4\pi\bar{J}} &= \frac{L_x^4 L_z}{a^5} \sqrt{\frac{t_y}{t_x}}, \\ \frac{\pi t_z}{2\bar{J}} &= \frac{L_x^2 L_z^3}{a^5} \sqrt{\frac{t_y}{t_x}}. \end{aligned} \quad (38)$$

Squaring the second equation in (38) and dividing the result by the first equation, we exclude L_x and obtain the following expression for L_z

$$L_z = a \left(\frac{\pi^3}{j_{0,1}^2 \bar{J}} \frac{t_z^2}{\sqrt{t_x t_y}} \right)^{1/5}. \quad (39)$$

Substituting Eq. (39) to the first equation in (38), we get

$$\frac{j_{0,1}^2 t_x}{4\pi\bar{J}} = \frac{L_x^4}{a^4} \sqrt{\frac{t_y}{t_x}} \left(\frac{\pi^3}{j_{0,1}^2 \bar{J}} \frac{t_z^2}{\sqrt{t_x t_y}} \right)^{1/5}. \quad (40)$$

Hence, we have

$$L_x = \frac{a}{\sqrt{2}} \left(\frac{j_{0,1}^3}{\pi^2 \bar{J}} \frac{t_x^2}{\sqrt{t_y t_z}} \right)^{1/5}. \quad (41)$$

Using Eqs. (39) and (41), we find volume Ω_{cyl} of the cylindrical ferron

$$\Omega_{cyl} = \pi \frac{L_x^2 L_z}{a^3} \sqrt{\frac{t_y}{t_x}} = \frac{(\pi j_{0,1})^{4/5}}{2} \left(\frac{t_x t_y t_z}{\bar{J}^3} \right)^{1/5}. \quad (42)$$

Introducing the effective hopping integral for the 3D case

$$t_{eff} = (t_x t_y t_z)^{1/3}, \quad (43)$$

we can rewrite Eq. (42) as

$$\Omega_{cyl} = \frac{(\pi j_{0,1})^{4/5}}{2} \left(\frac{t_{eff}}{\bar{J}} \right)^{3/5}. \quad (44)$$

Similar to the the 2D case, we see that the ferron volume in 3D is also a function of t_{eff}/\bar{J} ratio, where the effective parameters are given by Eqs. (37) and (43).

Substituting expressions (39), (41), and (44) for L_x , L_y , and Ω_{cyl} , respectively, to the energy of a FM polaron (35), we get

$$E_{pol} = 10n\bar{J}\Omega = 5n(\pi j_{0,1})^{4/5} (t_{eff}^3 \bar{J}^2)^{1/5} \quad (45)$$

We see that the polaron energy in the 3D case again depends on the universal parameters t_{eff} and \bar{J} , but the specific form of this dependence is slightly different: $(t_{eff}^3 \bar{J}^2)^{1/5}$ in 3D as compared to $(t_{eff} \bar{J})^{1/2}$ in 2D.

B. FM droplets of ellipsoidal shape

Here, we calculate the volume and the energy of the FM droplet having the ellipsoidal shape. The volume of the ellipsoidal droplet in the 3D case is

$$\Omega_{ell} = \frac{4}{3} \pi \frac{L_x L_y L_z}{a^3}. \quad (46)$$

In this case, the total energy of the system has the form

$$E_{tot} = -2 [t_x n + t_y n + t_z n + (J_x + J_y + J_z) S^2] + \varepsilon_0 n + 4(J_x + J_y + J_z) S^2 \Omega n. \quad (47)$$

Hence the energy of the elliptical FM polaron can be written as

$$E_{pol} = \varepsilon_0 n + 4\bar{J}\Omega n, \quad (48)$$

where we again introduce \bar{J} defined by Eq. (37).

As above, energy ε_0 can be found by solving the corresponding Schrödinger equation

$$\hat{H}_{kin} \Psi(x, y, z) = \varepsilon_0 \Psi(x, y, z), \quad (49)$$

where

$$\hat{H}_{kin} = -a^2 \left(t_x \frac{\partial^2}{\partial x^2} + t_y \frac{\partial^2}{\partial y^2} + t_z \frac{\partial^2}{\partial z^2} \right). \quad (50)$$

Using the the dilatation along the y and z axes: $\tilde{y} = y\sqrt{t_y/t_x}$ and $\tilde{z} = z\sqrt{t_z/t_x}$, we get

$$\hat{H}_{kin} = -t_x a^2 \Delta_{\tilde{R}} \quad (51)$$

in the 'new' coordinates x , \tilde{y} , and \tilde{z} . Here, we have $\tilde{R}^2 = x^2 + \tilde{y}^2 + \tilde{z}^2$ and $\Delta_{\tilde{R}} = \frac{\partial^2}{\partial \tilde{R}^2} + 2\frac{1}{\tilde{R}} \frac{\partial}{\partial \tilde{R}}$ is the radial part of the Laplacian operator in 3D.

In these coordinates, a droplet is confined within a sphere of radius $\tilde{R}_{max} = L_x$. Accordingly, we have

$$L_y \sqrt{t_x/t_y} = L_z \sqrt{t_x/t_z} = L_x = \tilde{R}_{max} \quad (52)$$

and the droplet volume expressed in terms of initial ('old') coordinates reads

$$\Omega_{ell} = \frac{4}{3} \pi \frac{L_x L_y L_z}{a^3} = \frac{4}{3} \pi \left(\frac{L_x}{a} \right)^3 \frac{(t_y t_z)^{1/2}}{t_x}. \quad (53)$$

A solution to the Schrödinger equation (49) has the form

$$\Psi(k\tilde{R}) = \frac{\sin(k\tilde{R})}{(k\tilde{R})}. \quad (54)$$

The boundary condition $\Psi(k\tilde{R}_{max}) = 0$ yields $k\tilde{R}_{max} = \pi$. Hence, we find

$$\varepsilon_0 = t_x a^2 k^2 = t_x a^2 \frac{\pi^2}{\tilde{R}_{max}^2} = t_x a^2 \frac{\pi^2}{L_x^2} \quad (55)$$

and the energy of ellipsoidal FM polaron takes the form

$$E_{pol} = t_x \frac{\pi^2 a^2}{L_x^2} n + 4\bar{J} n \frac{4}{3} \pi \left(\frac{L_x}{a} \right)^3 \frac{\sqrt{t_y t_z}}{t_x} \quad (56)$$

The minimization of polaron energy (48) with respect to L_x yields

$$\frac{\partial E_{pol}}{\partial L_x} = -2t_x \frac{\pi^2 a^2}{L_x^3} n + 16\bar{J}\pi n \left(\frac{L_x}{a} \right)^2 \frac{1}{a} \frac{\sqrt{t_y t_z}}{t_x} = 0 \quad (57)$$

As a result, we get the expression for L_x

$$L_x = a \left(\frac{\pi}{8\bar{J}} \frac{t_x^2}{\sqrt{t_y t_z}} \right)^{1/5}. \quad (58)$$

Substituting Eq. (58) to (59), we find the volume of an ellipsoidal droplet

$$\Omega_{ell} = \frac{\pi^{8/5} 2^{1/5}}{3} \left(\frac{t_{eff}}{\bar{J}} \right)^{3/5}, \quad (59)$$

where t_{eff} is again given by Eq. (43). We see that the volume of the ellipsoidal droplet is also determined by the dimensionless universal ratio t_{eff}/\bar{J} . Dividing Eq. (59) by Eq. (44), we obtain the ratio of volumes for ellipsoidal and cylindrical droplets

$$\frac{\Omega_{ell}}{\Omega_{cyl}} = \frac{4}{3} \left(\frac{\pi}{2j_{0,1}} \right)^{4/5} \simeq 0.95 < 1. \quad (60)$$

We see that the ellipsoidal FM droplet is a more compact object (with a smaller volume) than the cylindrical one.

Substituting expression (58) for L_x to the polaron energy (56), we find

$$E_{pol} = 10n\bar{J}\Omega_{ell} = 10n\frac{\pi^{8/5} 2^{1/5}}{3} (t_{eff}^3 \bar{J}^2)^{1/5}. \quad (61)$$

Hence the ratio of energies corresponding to two different shapes of ferrons is again identically equal to the ratio of their volumes

$$\frac{E_{pol}^{ell}}{E_{pol}^{cyl}} = \frac{\Omega_{ell}}{\Omega_{cyl}} = \frac{4}{3} \left(\frac{\pi}{2j_{0,1}} \right)^{4/5} \simeq 0.95 < 1. \quad (62)$$

Thus, in the 3D case, the ellipsoidal droplet has the lowest energy in agreement with the results of Ref. 3.

IV. CONCLUSIONS AND DISCUSSION

We considered the formation and the shape of droplets in the most general cases of doped anisotropic 2D and 3D

antiferromagnets with arbitrary values of the electron hopping integrals t_α and the AFM exchange integrals J_α . We found that in the anisotropic 2D case (when $\alpha = \{x, y\}$ and $t_x \neq t_y$, $J_x \neq J_y$), the most energetically favorable shape of FM droplets is an ellipse. In the anisotropic 3D case (when $\alpha = \{x, y, z\}$ and we include into consideration the third dimension with t_z and J_z), the most energetically favorable shape of FM droplets is an ellipsoid. Moreover, both the binding energy and the volume of FM droplets depend in the 2D as well as in the 3D cases upon only two universal parameters t_{eff} and \bar{J} . In the 2D case, these parameters are $t_{eff} = (t_x t_y)^{1/2}$ and $\bar{J} = (J_x + J_y) S^2$, whereas, in the 3D case, the corresponding expressions have the form $t_{eff} = (t_x t_y t_z)^{1/3}$ and $\bar{J} = (J_x + J_y + J_z) S^2$.

Note that in the present paper, we considered only the case of 'free' ferrons, which are not strongly localized at donor impurities. The study of strongly localized ferrons bound to impurities, especially their shape and the form of the cloud of magnetic distortions related to them (similar to those described in Refs. 9 and 17) will be the subject of a separate publication.

Note also that the situation would be more complicated for FM droplets in the frustrated triangular or kagome lattices. This is a case, for example, in an interesting quasi-1D magnetic material BaCoO_3 , where the chains of Co^{4+} ions form a triangular lattice^{6,7}.

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